A Phenomenological Description of the Non-Fermi-Liquid Phase of MnSi *

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In order to understand the non-Fermi-liquid behavior of MnSi under pressure we propose a scenario on the basis of the multispiral state of the magnetic moment. This state can describe the recent critical experiment of the Bragg sphere in the neutron scattering which is the key ingredient of the non-Fermi-liquid behavior.

Key Words: **MnSi, non Fermi liquid, nesting, helimagnet, multispiral, Bragg sphere**

MnSi is one of the most extensively studied materials from the viewpoint of itinerant magnetism. Recently its non-Fermi-liquid (NFL) nature [1–3] which can not be understood within the standard theory [4–6] has been reported. We will give a phenomenological description of this NFL behavior in this Short Note as a starting point for constructing a microscopic theory.

MnSi is a helimagnetic metal at ambient pressure for the temperature T below the transition temperature $T_{\rm c} = 29.5$K. $T_{\rm c}$ is suppressed by the application of hydrostatic pressure p and vanishes at the critical pressure $p_{\rm c} = 14.6$kbar. For $T > T_{\rm c}$ MnSi is a paramagnetic metal. The phase transition changes its character at $p = 12\text{kbar} \equiv p^*$. For $p < p^*$ the transition is of second order, while for $p > p^*$ it is of weakly first order. It should be noted that a crossover line $T = T_0(p)$, which merges to the transition line $T = T_{\rm c}(p)$ at $p = p^*$, exists in $p - T$ plane. For $T_{\rm c} < T < T_0$ the local magnetic moment exists even in the paramagnetic phase. Here $T_{\rm c} = 0$ for $p > p_{\rm c}$. These behaviors in $p - T$ plane are summarized, for example, in Fig. 1 of ref. 3.

The NFL behavior in the DC resistivity [1,2] is observed roughly for $T_{\rm c} < T < T_0$ as stated in the caption of Fig. 3 in ref. 3. In this region the resistivity R is proportional to $T^{3/2}$. For $p > p_{\rm c}$ where $T_{\rm c} = 0$ this fractional power dependence persists down to a few mK. This behavior is unexpected in two points. Firstly the transition at $T_{\rm c}$ is of first order for $p^* < p < p_{\rm c}$, while such a fractional power dependence is expected near the second order transition. Secondly there is no characteristic scale of temperature in the resistivity for $p > p_{\rm c}$, while such a vanishing of the scale is expected only at the critical pressure of the second order transition.

In order to understand the NFL behavior a critical experiment by neutron scattering has been reported very recently. [3] Across the first order phase transition line in $p - T$ plane the unlocking of the spiral occurs. Namely, it is observed that the scattering intensity in the paramagnetic phase spreads around the Bragg sphere of radius $Q \sim 0.043\text{Å}^{-1}$ in reciprocal lattice space, while in the long-range ordered helimagnetic phase at ambient pressure the magnetic Bragg peak is observed at the point of $\vec{Q} = 0.037\text{Å}^{-1}(1, 1, 1)$ which specifies the spiral of the magnetic moment in real space.

On the basis of this neutron scattering experiment we try to explain the NFL behavior in the temperature dependence of the resistivity in a phenomenological manner. Firstly we discuss the nature of the transition. For $p < p^*$ the transition at $T = T_{\rm c}$ is a simple spin-density wave formation. The local moment is absent for $T > T_{\rm c}$ in this pressure range and the transition is of second order. For $p > p^*$ non-vanishing global order parameter is attained only for $T < T_{\rm c}$, while the local moment is formed for $T < T_0$. In the region $T_{\rm c} < T < T_0$ a quasi-long-range correlation is developed, although the global order parameter vanishes. Since the local moment is already formed for $T > T_{\rm c}$, the transition at $T = T_{\rm c}$ becomes first order in this pressure range. The driving force for the global order is weak and the transition is of weakly first order.

As an candidate for the driving force we can think of the nesting of the Fermi surface, since such a weak global effect arises from the low-energy states around the Fermi energy. Some nesting tendency of the Fermi surface is seen in the band calculation. [7,8] It is naturally expected that the preferred direction of the spiral is determined by the nesting vector. In the magnetically ordered state the Fermi surface is gapped around the Bragg wave-vector. The wave vector is determined by the nesting of the Fermi surface. The gap is formed to gain the potential energy in spite of the kinetic energy loss. By the application of hydrostatic pressure the relative importance of the kinetic energy increases and the gap collapses at $T = T_{\rm c}$. Across the first-order transition for $p > p^*$ the Bragg peak in the neutron scattering intensity spreads over the Bragg sphere. This unlocking of the spiral occurs in order to gain kinetic energy.

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The dissociation of T_c and T_0 for $p > p^*$ results from the fluctuation of the magnetic moments due to the kinetic energy.

It should be noted that the absence of inversion symmetry in MnSi related to B20 crystal structure is one of the most important features of this material. The helimagnetism is discussed to be derived from the Dzyaloshinsky-Moriya interaction allowed for this symmetry from the view point of localized magnetic moments. [9,10] On the other hand, MnSi is well described as an itinerant magnet [5,11] so that the same effect is realized in the renormalized band structure for quasiparticles. Namely, the electronic state of MnSi is described as a Fermi liquid with a quasiparticle band into which the effect of localized magnetic moments are renormalized. [11] The renormalized quasiparticle band has nesting tendency. [7,8] Since we are interested in the low-temperature behavior around the quantum critical point, the approach on the basis of the Fermi liquid is more appropriate than that on the basis of the localized magnetic moments.

Since a formation of the Bragg circle has been theoretically reported in a two-dimensional case on the basis of a double spiral state [12,13] where the spiral of the magnetic moment is specified by two basis vectors, we expect that the Bragg sphere is derived from some multispiral state. The microscopic derivation of the multispiral state needs detailed information on the Fermi surface and should be done in a future study. The absence of the characteristic temperature even in the region away from the quantum critical point can be understood by the mechanism of the gradual change of the wave vector specifying the multispiral state, while the nesting vector specifying the Bragg peak is uniquely defined. Thus in the wide range for $p > p_\mathrm{c}$ the coherence length becomes divergently large on the Bragg sphere in the limit of $T \to 0$. In this paper we use the word, the coherence length, after ref. 3 and it should be distinguished from the true correlation length as discussed below. The microscopic derivation of the above mechanism on the basis of the gradual change of the Fermi-surface shape should be also done in a future study.

Next we discuss the NFL nature observed in the temperature dependence of the resistivity. In the wide region of interest, $p > p_\mathrm{c}$, the coherence length can be assumed to be divergently large [3] in the limit of $T \to 0$. Thus the coherence length ξ is approximately modeled as

$$\xi^{-2} \sim \alpha T, \tag{1}$$

where the right-hand-side term is induced by the mode-mode coupling [5,6] and α is a temperature-independent constant. This form is derived for non-critical state, while we have approximately set $\xi^{-2} \to 0$ when $T \to 0$ in consistent with the resolution-limited scattering intensity. [3] With this ξ the imaginary part of the dynamical spin susceptibility at low energy can be modeled as

$$\chi''(\vec{q},\omega) = \frac{D\omega/\Gamma}{[\xi^{-2} + A(\vec{q}-\vec{Q})^2]^2 + (\omega/\Gamma)^2}, \tag{2}$$

where $\vec{Q} = Q(1,1,0)$ with $Q \sim 0.043\text{Å}^{-1}$. A and D are constants independent of $\vec{q}$, ω and T. Here we have taken into account the fact that the notion of the Bragg sphere is an approximate one and that the scattering intensity is strongest at this $\vec{Q}$ as observed in the experiment. [3] The parameter for the dissipation Γ is of the order of $v_\mathrm{F}Q$ where v_F is the renormalized Fermi velocity for quasiparticles. This form is valid at low energy of $\omega < \Gamma$ and sufficient for the discussion of the low-temperature behavior of the resistivity.

It should be noted that the coherence length ξ used in this paper is effective only for the modeling of the imaginary part of the susceptibility at low energy of $\omega < \Gamma$. Actually the divergent behavior in the neutron scattering intensity [3] is related to the imaginary part of the susceptibility in the low-energy limit. The true correlation length or the thermodynamic susceptibility is determined by the real part, $\chi(\vec{q})$ at $\omega = 0$, which is related to the imaginary part by the Kramers-Kronig relation as $\chi(\vec{q}) = \frac{1}{\pi}\int_{-\infty}^{\infty}\mathrm{d}\omega\chi''(\vec{q},\omega)/\omega$. The behavior of the true correlation length is determined not only by low-energy process but also by high-energy process and does not necessarily coincide with the coherence length characterizing the low-energy behavior. Such a situation is similar to the case of cuprate superconductors. [14]

Using this $\chi''(\vec{q},\omega)$ of $z = 2$ form, where z is the dynamical exponent, we calculate the resistivity R. It is easily evaluated for our non-critical state as a correction to the Fermi-liquid behavior [15] as

$$R \propto T^2 \sum_{\vec{q}} \frac{1}{[\xi^{-2} + A(\vec{q}-\vec{Q})^2]^2}. \tag{3}$$

Here the extracted factor T^2 represents the Fermi-liquid behavior and is consisitent with the form of the dissipative term ω/Γ in $\chi''(\vec{q},\omega)$. The summation in the right-hand side representing the correction is proportional to the integral

$$\int_0^{p_\mathrm{c}} \frac{p^2\mathrm{d}p}{(p^2+\xi^{-2})^2} \sim \xi \sim (\alpha T)^{-1/2}, \tag{4}$$

where we have set as $\vec{p} = \sqrt{A}(\vec{q} - \vec{Q})$. Thus we obtain

$$R \propto T^{3/2}, \tag{5}$$

in the low-temperature limit. This form of resistivity scaling is valid for $T < \Gamma$ where the assumed form of $\chi''(\vec{q}, \omega)$ is dominant in the evaluation of the resistivity. Since $v_{\rm F}$ and Q depend only weakly on the applied pressure, the crossover temperature $\tilde{T} \equiv \Gamma$ also depends only weakly on the pressure in consistent with the experiment. [1–3]

In this Short Note we have proposed the multispiral state in order to explain the key experiment of the Bragg sphere in the neutron scattering. A microscopic description of such a state needs detailed information on the Fermi surface and is left as a future study. On the basis of the quasi-long-range correlation observed as the Bragg sphere the NFL behavior in the temperature dependence of the resistivity is naturally understood.

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